IMPORTANT NOTICE: The current official version of this document is available via the Sandia National Laboratories NWMP On-line Documents web site. A printed copy of this document may not be the version currently in effect.

Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Plan for Testing a Refined BRAGFLO Grid for the Technical Baseline Migration (TBM)

AP-082

Task Number
1.3.5.1.2.3

Effective Date: 01/07/02

Author: Joshua S. Stein (6821) *Original signed by Joshua S. Stein* *12-17-01*
Print Signature Date

Author: Teklu Hadgu (6821) *Original signed by Teklu Hadgu* *12/17/01*
Print Signature Date

Technical
Review: James Schreiber (6852) *Original signed by James D. Schreiber* *12/12/2001*
Print Signature Date

Management
Review: Kathryn Knowles (6821) *Original signed by M.K. Knowles* *12-21-01*
Print Signature Date

QA Review: Mario Chavez *Original signed by Mario Chavez* *1/7/02*
Print Signature Date

TABLE OF CONTENTS

LIST OF TABLES

1.0 INTRODUCTION AND OBJECTIVES

This analysis plan describes plans to test a new two-dimensional BRAGFLO computational grid. This grid incorporates a number of changes that are proposed for the upcoming Technical Baseline Migration (TBM) calculations. The TBM is an effort to merge CCA (U.S. DOE, 1996) and PAVT (PAVT, 1997) baselines while at the same time implement changes that are explained in Wall, 2001. The most important change with respect to repository fluid flow is the removal of the shaft seal from the BRAGFLO grid. Making this change to the grid requires the recalculation of the z dimensions for the grid cells. The z dimension is assigned so that the two-dimensional grid simulates three-dimensional flow away from or towards the repository. One goal of this analysis plan is to describe the method we use to recalculate the z dimensions. In addition to removing the shaft from the grid, we have also refined the grid spacing in several parts of the grid. These additional changes are intended to reduce the large numerical dispersion observed in these areas for previous calculations. It is not in the scope of this test plan to quantify to what degree we have reduced numerical dispersion, but instead to test whether the proposed grid changes significantly affect BRAGFLO results for a sample of CCA and PAVT vectors. The test will comprise running the new grid with parameters chosen from specific PA vectors from the CCA and the PAVT. The final grid that is planned for the TBM will include all of the changes tested here, but will also include changes that are not directly comparable to previous grids because of changes to the repository design (Option D panel closures), and conceptual model changes (Disturbed Rock Zone). All of the proposed changes will be presented in front of a peer review panel and will be summarized in a future analysis plan describing the Salado flow and transport calculations to be conducted for the TBM.

2.0 APPROACH

The CCA grid had (NX, NY) dimensions of (33, 31). The new grid has dimensions (68, 33) The specific changes that will be implemented for this comparative study are as follows:

1. Shaft is removed.
2. *x*-spacing of the grid beyond the repository to the north and south is refined.
3. Layers above and below Marker Bed 139 have been made relatively thin (~1 m thick) and y grid spacing in Salado has been changed.
4. Repository representation is redefined as described below.

2.1 Assumptions for the new grid

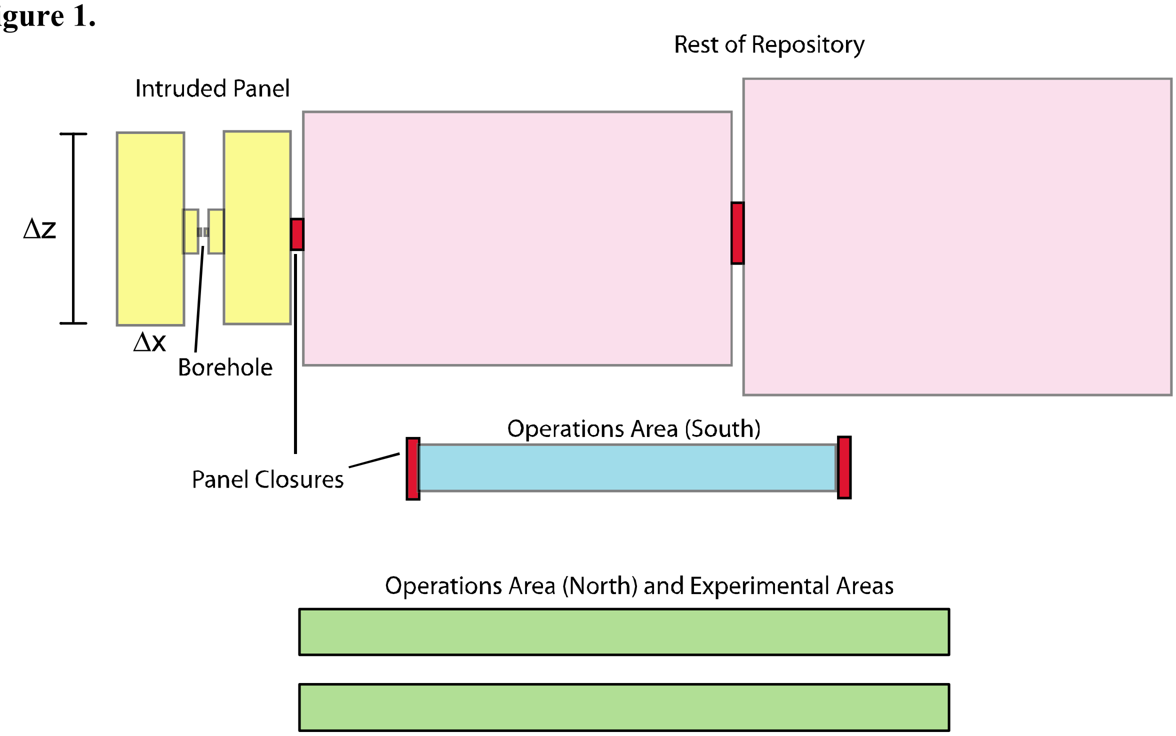
1. Volumes used for the CCA grid are accurate for the following regions:
    a. Intruded panel (4.61635×10^4 m^3)
    b. Rest of repository (3.89981×10^5 m^3)
    c. Operations + Experimental + Panel closure (PCS) areas = (1.42966×10^5 m^3)

2. Excavated area *x*-length (north-to-south) from the CCA grid is appropriate (1829.89m).

2.2 The repository horizon

1. The excavated areas (intruded panel, rest of repository (RoR), panel closures (PCS), operations and experimental areas are defined such that the total excavated volume is equal to that modeled in the CCA. The extent of several regions has been modified. Starting from the south end of the repository and moving north the following regions will be defined (Figure 1):
    a. Intruded panel (representing either panel 4 or 5) [7 *x*-divisions]
    b. PCS (representing two PCS's) [2 *x*-divisions]
    c. Southern RoR (representing panels 3, 6, 9 and either 4 or 5) [2 *x*-divisions]
    d. PCS (representing four PCS's) [2 *x*-divisions]
    e. Northern RoR (representing panels 1, 2, 7, 8, and 10) [2 *x*-divisions]
    f. PCS (representing four PCS's) [2 *x*-divisions]
    g. Southern operations area [2 *x*-divisions]
    h. PCS (representing four PCS's) [2 *x*-divisions]
    i. Northern operations and experimental areas [2 *x*-divisions]

Figure 1.



2. "Rectangular" flaring occurs at two spatial scales:
    a. <u>Borehole scale:</u> around the borehole in the intruded panel the grid will flare as in the CCA. This flaring (Δz) is not changed from the CCA (Figure 1).

b. Regional scale: beyond the excavated area to the north and south the grid will flare to represent divergent flow away from or toward the waste filled part of the repository. Rectangular flaring is implemented so that the grid represents all the volume around the excavated areas. See next section for details.

The grid blocks to the north and south of the excavated region will be refined in the *x*-direction from the CCA baseline. The *x*-dimension of the grid will increase by a factor of 1.45 to the north and south of the excavated region except at the location of the Land Withdrawal Boundary and the far ends of the grid where grid spacing was adjusted to accommodate specific analyses of model results. This refinement factor was chosen so that starting with a horizontal grid spacing of 2 m directly outside the excavated area there would be approximately twice the number of grid cells (68) for a grid that was the same overall size as the CCA grid. In the y direction the grid spacing within layers representing the Salado has been changed from the CCA. The CCA grid spacing in this region was dictated by the thickness of different shaft seal materials. Since we are no longer representing the shaft in the model, we have regularized the *y* spacing in these regions. In addition, we have added two layers so that we could refine the grid spacing in the layers immediately surrounding Marker Bed 139. This results in a total of 33 *y*-divisions for the grid. A picture of the logical grid is included at the end of this analysis plan (Figure 3).

2.3 Rectangular flaring scheme

The regional rectangular flaring occurs *only* for the grid blocks to the north and south of the excavated region. The flaring is similar to what was done for the CCA grid, but simpler (Figure 2). Looking from the top of the grid (*x*-*z* plane), consider that the excavated region is now represented by a rectangle of length x = 1830 m and width z = 80 m, we call this East-West distance, D_{EW}. This simplification maintains the area (and volume) of the actual gridded excavated region for the calculation of the Δz's needed to represent flaring. In order to calculate the rectangular flaring we need to choose a center line to divide the flaring on the north and south. Because the waste panels are located in the southern part of the excavated area, we choose the "center of waste" as the middle of the PCS that separates the northern RoR from the southern RoR. We define the position of this "center of the waste" by the distances from the north and south edges of the gridded repository, D_N and D_S, respectively. {D_N = 1378 m, D_S = 452 m, $D_N + D_S$ = 1830 m} Each flared grid block has length, Δx, and width, Δz. The block can be thought of as wrapped around the excavated area like half a rectangular onion, with the center at the center of waste (Figure 2). Each Δz can be calculated from the preceding Δx's as follows.
For the northern end:

$$\Delta z_1 = 2D_N + D_{EW} + 2\Delta x_1$$

$$\Delta z_2 = 2D_N + D_{EW} + 4\Delta x_1 + 2\Delta x_2$$

$$\Delta z_3 = 2D_N + D_{EW} + 4\Delta x_1 + 4\Delta x_2 + 2\Delta x_3$$

.

.
.

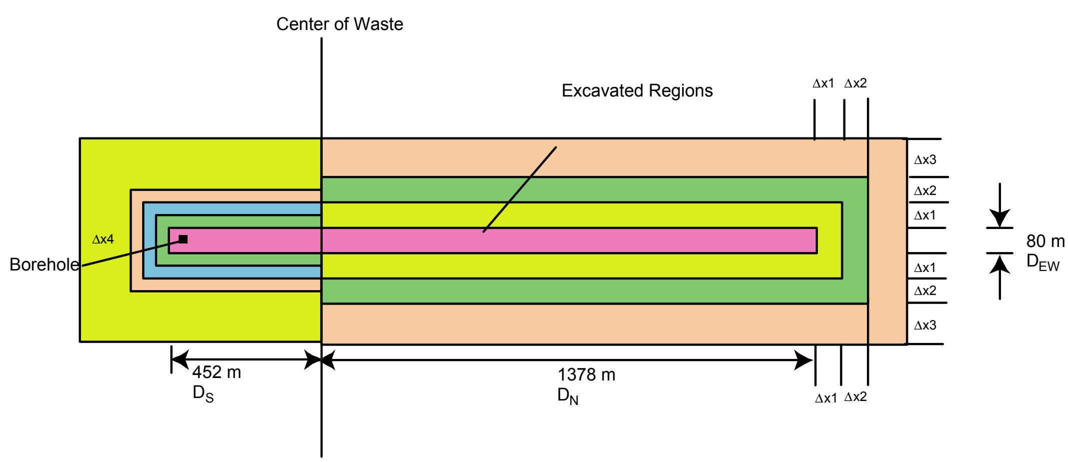
$$\Delta z_n = 2D_N + D_{EW} + 4\sum_{i=1}^{n-1}\Delta x_i + 2\Delta x_n$$

Southern end is the same with D_S substituted for D_N.

This method of rectangular flaring ensures that the grid accounts for all the volume surrounding the repository.

Figure 2.

TBM BRAGFLO Grid
Simplified Rectangular Flaring



3.0 TEST STRATEGY

We will run BRAGFLO for 20 selected CCA and PAVT vectors (10 vectors from each). Then we will run the same vectors using the new grid for a total of 40 BRAGFLO runs. Time histories of pressure and saturation in the repository will be plotted against the results from the appropriate comparison vectors. Cumulative brine flow into and out of the repository will also be compared. The CCA and PAVT vectors that will be used for the comparison are listed in Table 1. A similar grid comparison was performed by Shortencarier et al. (1998) to test the adequacy of the ASA98 grid.

Table 1. CCA and PAVT vectors for grid comparison.

Vector →	***1***	***2***	***3***	***4***	***5***	***6***	***7***	***8***	***9***	***10***
CCA R1	S1-37	S2-20	S3-30	S4-40	S5-50	S6-60	S1-70	S2-80	S3-90	S4-100
PAVT R1	S1-26	S2-28	S1-38	S3-58	S4-51	S5-2	S6-5	S1-70	S2-80	S3-90

4.0 SOFTWARE LIST

The software versions to be used for this grid test are listed below in Table 2.

Table 2. Software List

Code	***Version***
ALGEBRACDB	2.35
BRAGFLO	4.10.02
GENMESH	6.08
ICSET	2.22
MATSET	9.04
POSTBRAG	4.00
PREBRAG	6.10
SPLAT	1.02
SUMMARIZE	2.20

Software Steps:

1. The new grid will be constructed using GENMESH.
2. MATSET will be run next to select the proper variables from the PA database.
3. Next the files, "LHS2_BF_CCA_TRN_R1.OUT" and "LHS2_BF_C97_TRN_R1.OUT" will be retrieved from the Configuration Management System (CMS) and POSTLHS will be run to generate a full R1 replicate of CAMDAT (.CDB) files from the CCA and PAVT for the new grid.
4. Next ICSET will be run on vectors listed in the comparison Table 1.
5. ALGEBRA and then PREBRAG will be run to produce BRAGFLO input files. We are using PREBRAG version 6.10, which is not currently qualified, but we are actively in the process of getting this version qualified.

6. Minor changes will need to be made to the file "PARAMS.INC" and BRAGFLO will need to be recompiled to accommodate the larger dimensions of the new grid. BRAGFLO will be run.
7. BRAGFLO output will be processed with POSTBRAG, ALGEBRA, and SUMMARIZE, and then plots will be produced using SPLAT.

5.0 TASKS

Joshua Stein will design the new grid, set up the appropriate input files, and run the necessary BRAGFLO simulations. Teklu Hadgu will provide experience and support as needed. Roger Coman will provide support for the CMS. Steve Tisinger will provide PA parameter database support. Joshua Stein will compile results and submit a report by April 1, 2002.

6.0 SPECIAL CONSIDERATIONS

No special considerations have been identified for this analysis.

7.0 APPLICABLE PROCEDURES

Analyses will be conducted in accordance with the quality assurance (QA) procedures listed below.

Training: Training will be performed in accordance with the requirements in NP 2-1, Qualification and Training.

Parameter Development and Database Management: Selection and documentation of parameter values will follow SP 9-1. The database is to be managed in accordance with relevant technical procedure.

Computer Codes: New or revised computer codes that will be used in the analyses will be qualified in accordance with NP 19-1. All other codes unchanged since the PAVT to be qualified under multi-use provisions of NP 19-1. The platform on which the codes will be run is the Compaq Alpha, Open VMS AXP, Version 7.2-1.

Analysis and Documentation: Documentation will meet the applicable requirements in NP 9-1.

Reviews: Reviews will be conducted and documented in accordance with NP 6-1 and NP 9-1, as appropriate.

8.0 ACRONYMS

CMS	Configuration Management System
TBM	Technical Baseline Merger
CCA	Compliance Certification Application
PAVT	Performance Assessment Verification Test

9.0 REFERENCES

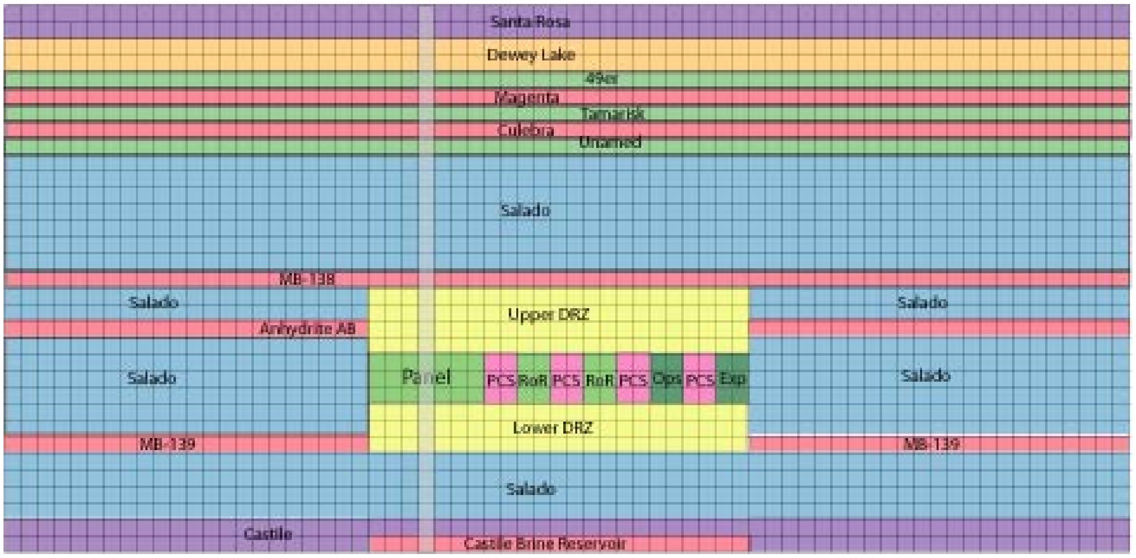
Shortencarier, M., A. Treadway, and J. Bean, 1998, Analysis documentation for testing the adequacy of the grid used for the BRAGFLO computer code calculations for the 1998 annual sensitivity analysis, WPO#51271 cross-referenced to WPO#49185.

PAVT, 1997, Supplemental Summary of EPA-Mandated Performance Assessment Verification Test (All Replicates) and Comparison with the Compliance Certification Application Calculations, WPO# 46702, Report # 414879.

U.S. DOE (U.S. Department of Energy), 1996, Title 40 CRF Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant. DOE/CAO-1996-2184.

Wall, D., 2001, Technical Baseline Migration Analysis Plan AP-075, ERMS# 519385.

Figure 3.


Santa Rosa
Dewey Lake
49er
Magenta
Tamarisk
Culebra
Unnamed
Salado
MB-138
Salado
Upper DRZ
Salado
Anhydrite AB
Salado
Panel
PCS
RoR
PCS
RoR
PCS
Ops
PCS
Exp
Salado
Lower DRZ
MB-139
MB-139
Salado
Castile
Castile Brine Reservoir